Elongation Control in an Algorithmic Chemistry

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Problem

- **Algorithmic chemistries** can be **constructive**: they produce new molecular species, e.g. strings, which can grow arbitrarily long (like bloat in genetic programming).
- Such **elongation** helps exploring the search space, but may also hinder the evolution of efficient functions and slow down the simulation.

Solution: Energy Control

- **Energy control** allows evolution to find solutions where molecule lengths are optimized.
- The solutions achieve a compromise between **conciseness** and exploration of **complexity**.

String Rewriting Chemistry

- We deliberately created a chemistry where molecules aggressively elongate.
- Molecules are strings of arbitrary length over an alphabet **{A,M,s,n}**
- The head symbol defines the string rewriting operation:

$$
\begin{array}{lll}
\mathbf{A}\Psi + \mathbf{M}\Omega & \rightarrow \Psi\Omega & \text{(join)} \\
\mathbf{s}\alpha\beta\Omega & \rightarrow \alpha\Omega + \beta\Omega & \text{(split)} \\
\mathbf{n}\Omega & \rightarrow \Omega & \text{(neutral)}
\end{array}
$$

α,β: symbols; Ψ,Ω: strings

An Energy Framework: Microscopic Reactions Yield Macroscopic Thermodyn. Behavior

Our reaction algorithm:

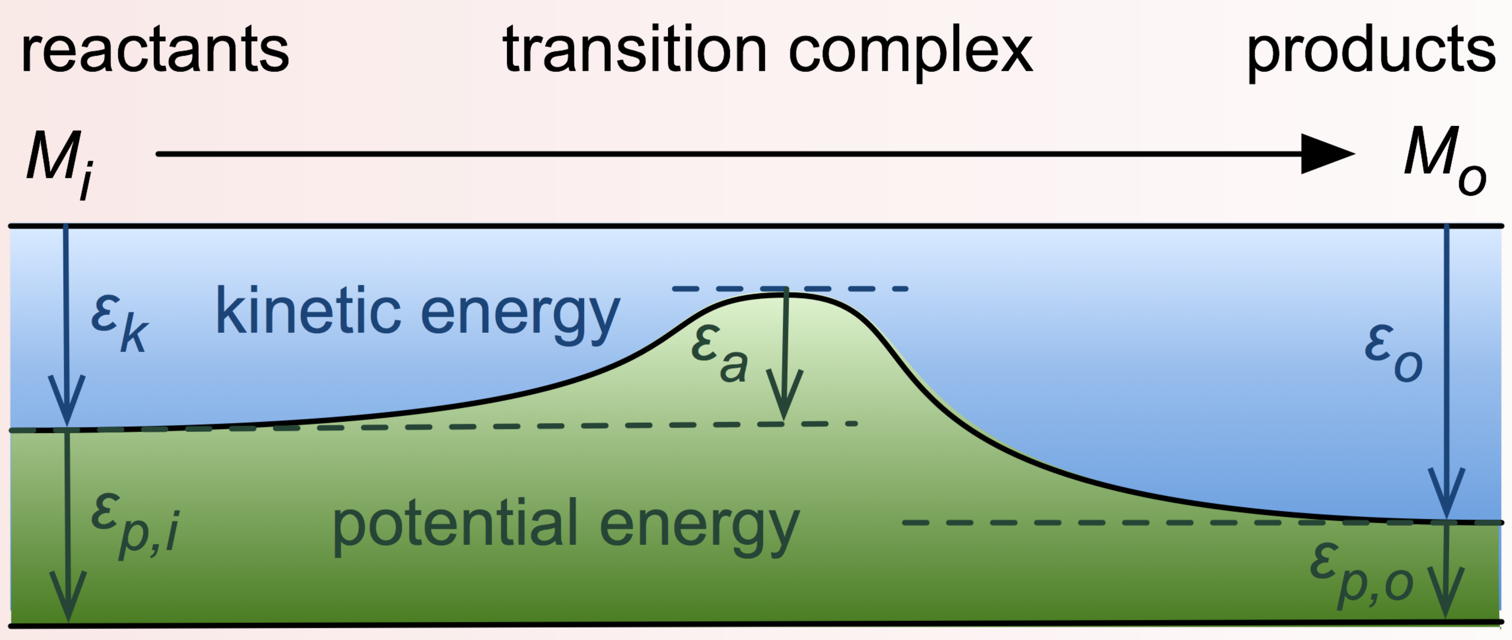
1) Collide: Select reactants (e.g. using Gillespie)

2) React: Decide whether a reaction is effective:

a) Draw a random collision energy from the kinetic energy pool E_k (N: number of molecules)

$$\varepsilon_k \sim Exp(E_k/N)$$

b) React if it exceeds the activation energy: $\varepsilon_k > \varepsilon_a$



3) Conserve Energy: Release the remaining kinetic energy back to the pool: $\varepsilon_o = (\varepsilon_k + \varepsilon_{p,i}) - \varepsilon_{p,o}$

Evolution Experiments: Only an incorporation of energy prevents uncontrolled elongation

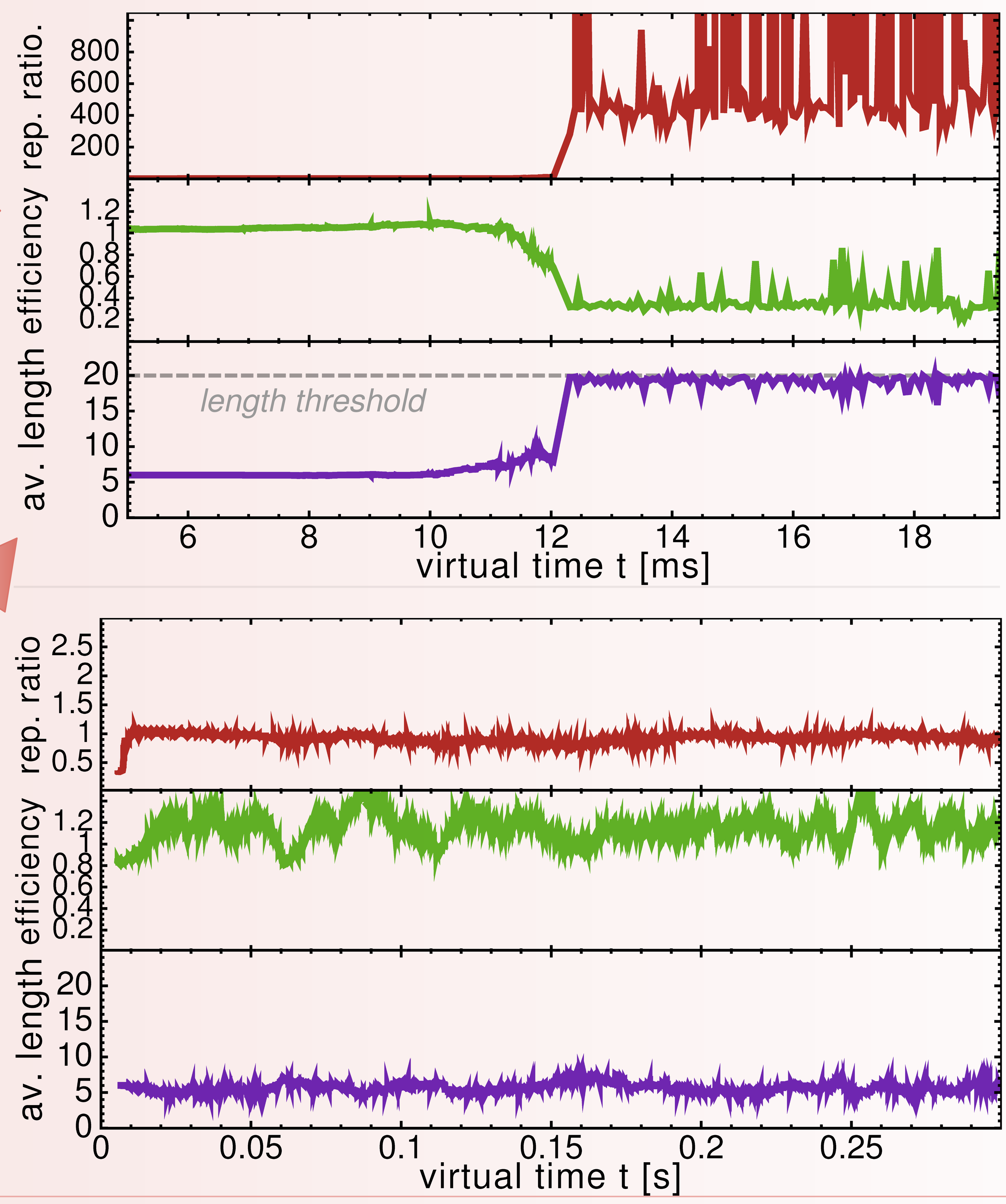
Setup: A population of 100 vessels ("**cells**") containing trivial self-replicators **{AsssAM, MsssAM}** evolves as cells grow, divide and mutate.

Summary

We evolved replicators in three different setups:

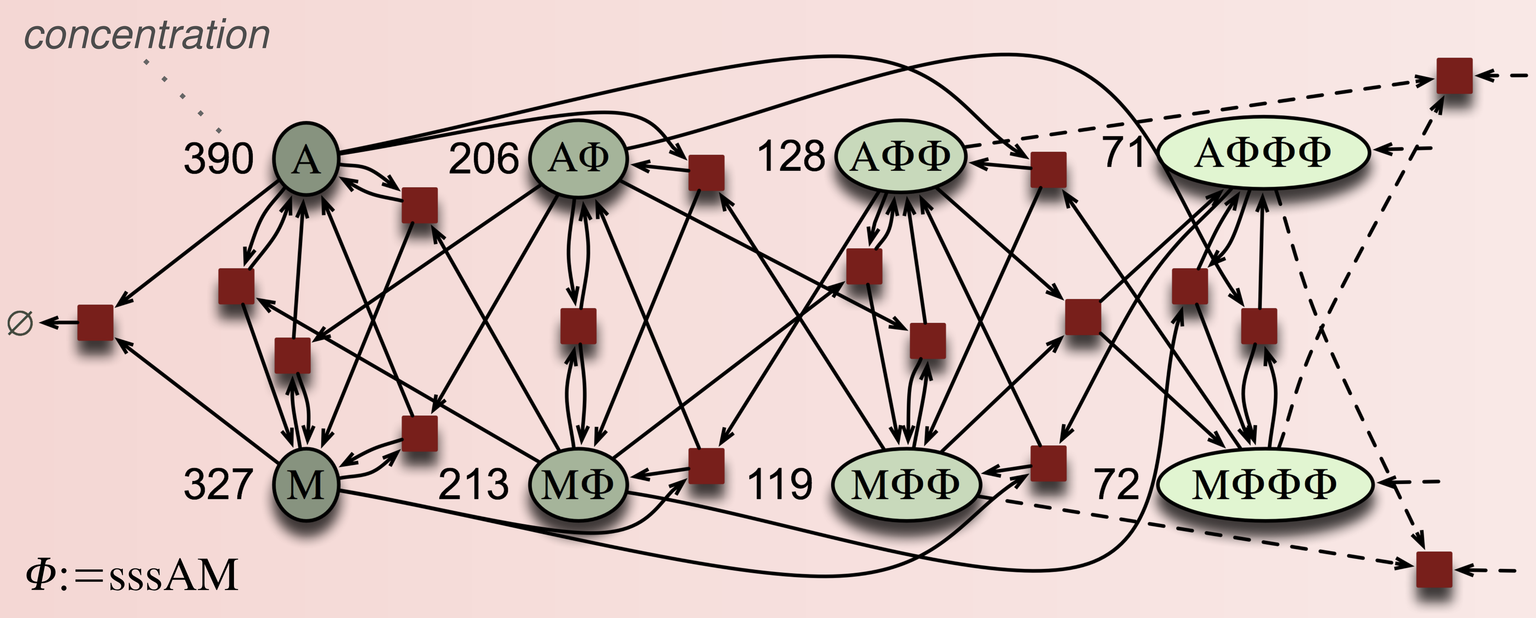
- **No constraints**: Unbounded elongation observed.
- **Destroy or truncate molecules** larger than a threshold: Prevents elongation but is inefficient.
- Our **energy framework**: Efficient control of molecule lengths; emergence of cooperating clusters.

Simulation Results



Emergence of cooperating clusters

With our energy model, the original self-replicators often **evolved to clusters** of molecules, which all react among each other; their concentration exponentially decreases with their length.



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